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Temperature determination using K_α spectra from M-shell Ti ions

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The Compact Multipulse Terawatt (COMET) laser facility at LLNL was used to irradiate Al-coated 2 – 50 μm Ti foils with $\approx 4 \times 10^{18} \text{ W cm}^{-2}$, 500 fs, 3 – 6 J laser pulses. Laser-plasma interactions on the front side of the target generate hot electrons with sufficient energy to excite inner-shell electrons in Ti, creating K_α emission which has been measured using a focusing spectrometer with spatial resolution (FSSR-1D) aimed at the back surface of the targets. The spatial extent of the emission varies with target thickness, and the high spectral resolution ($\lambda/\Delta\lambda \approx 3800$) is sufficient to measure blue shifts in K_α arising from ionization of near-solid Ti into the 3p subshell. A self-consistent-field model is used to spectroscopically diagnose thermal electron temperatures up to 40 eV in the strongly coupled Ti plasmas.

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At the extremes of ionization, K_α radiation is a well-studied phenomenon. Neutral atoms fluoresce when bombarded by photons, electrons, or ions with sufficient energy to excite or ionize a 1s inner-shell electron, emitting characteristic K_α radiation when a 2p electron decays to fill the 1s vacancy. The energies and fluorescence yields of such K_α transitions have been widely tabulated [1–3]. At the other extreme of ionization, the resonance 1s – 2p transitions in H- and He-like ions and their Li-like satellites have also been extensively studied and are foundational for spectroscopic plasma diagnostics [4, 5].

Due to reduced screening of the ion charge with increasing ionization, K_α transitions tend to undergo blue shifts as successive electrons are removed. The shifts are largest under the removal of inner-shell electrons and are relatively small when valence electrons are removed. Even small red shifts can occur under ionization for a few near-neutral species of transition metals; these anomalous shifts were first predicted by House [2] and later observed in high resolution measurements of Ni and Fe K_α emission from vacuum spark plasmas [6, 7].

Measurements of characteristic K_α yield have been powerful diagnostics for laser plasmas [8–10], where their high transition energies help to isolate the effects of hot electrons formed by laser-plasma interactions from the effects of thermal processes. In 1980, Duston *et al.* suggested that spectroscopic K_α (rather than K_α yield) measurements could be used to characterize the warm, dense material formed on the back surface of laser-irradiated foils [11]. Time-resolved K_α spectra from Al and Ti foils irradiated by a $3 \times 10^{14} \text{ W/cm}^2$ laser were subsequently measured [12]: streak-camera spectra showed burnthrough from neutral to H-like Al and Mg-like Ti, but no temperature information was extracted. In 1993, time- and space-integrated spectra were collected from the front (*i.e.* laser-irradiated) surface of Al-coated Si foils heated by $3 \times 10^{15} \text{ W/cm}^2$, 1.3 ps laser pulses [13]. The measured K_α emission from Li- to O-like Si under

various thicknesses of Al were used to infer a temperature profile for the Si substrate. More recently, K_α emission from L-shell Cl ions was used to infer temperatures near 100 eV near the surface of chlorinated plastic targets irradiated by 10^{17} W/cm^2 , 130 fs laser pulses [14].

Outside of the widespread diagnostics based on spectroscopy of H- to Li-like ions, the use of K_α spectra as a plasma diagnostic has, to our knowledge, been largely limited to analysis of the relatively well resolved K-shell lines from L-shell ions (*e.g.* [13–16]). Diagnostics based on spectroscopically resolved K_α emission from M-shell ions are not yet well developed but are of particular interest in the study of warm, dense matter – a necessary transitional state between the well studied solid-state and plasma regimes – where mid- Z elements are only a few times ionized. The warm, dense matter regime overlaps with the strongly coupled plasma regime (of particular interest in inertial confinement fusion studies), where the Coulomb interaction energy between ions exceeds the thermal kinetic energy of electrons. In this paper, we present K_α emission measurements with spatial and high spectral resolution from M-shell Ti ions and introduce a model that can extract thermal temperatures from the measured spectra.

The experiments were conducted on the Compact Multipulse Terawatt (COMET) laser at the Lawrence Livermore National Laboratory [17], a hybrid Chirped Pulse Amplification (CPA) system consisting of a Ti:Sapphire oscillator and regenerative amplifier tuned to 1054 nm wavelength with a 4-stage Nd:phosphate glass amplifier. To obtain the present data, 3 – 6 J of laser energy were delivered to the target in a 500 fs pulse, which was focused by an off-axis parabola to a spot size of $\approx 10 \mu\text{m}$ FWHM at an incident angle of 45° . The nominal laser intensity reached a few times $10^{18} \text{ W cm}^{-2}$, and the contrast of the laser pulse (the ratio between the peak intensity and the intensity 5 ps before the peak) was about 10^6 . The targets were Ti foils between 2 and 50 μm thick and were

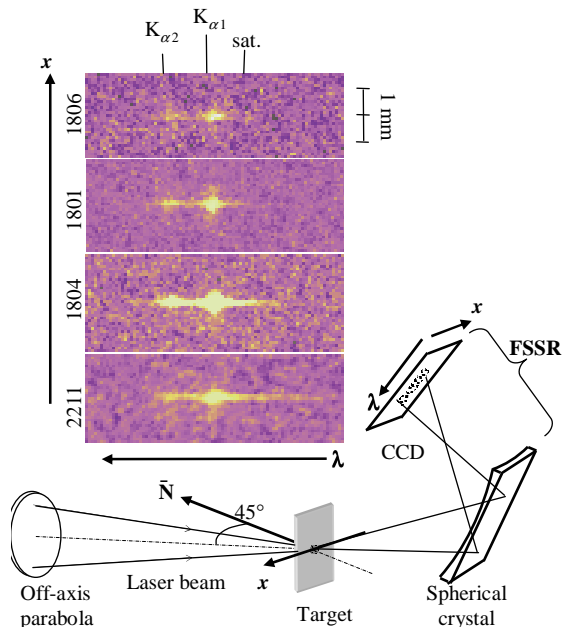


FIG. 1: (Color online) Scheme of experimental setup and images from four shots obtained by the FSSR spectrometer from the back surface of Al-coated Ti targets.

coated on the front (laser-irradiated) surface with 1000 Å of Al. The Al coating absorbs the small amount of energy in the laser prepulse, prevents direct laser heating of the Ti target, and acts as a tamper to the Ti foil over the short duration of the main laser pulse. The tamping ensures that the back surface of the targets remains near solid density over the few-ps time scale of K_α emission (as measured by a time-resolved Von Hamos spectrometer aimed at the front of the targets).

Spatially resolved x-ray spectra were measured using a focusing spectrometer with spatial resolution (FSSR-1D) [18, 19] equipped with a spherically bent quartz crystal ($R=150$ mm, $2d_{21\bar{3}0} \approx 3.082$ Å) and a vacuum compatible back illuminated CCD camera. The spectrometer viewed the back surface of the target at an angle of $\approx 30^\circ$ to the horizontal and $\approx 20^\circ$ to the vertical relative to the laser axis (see Fig. 1). For observation of the K_α spectral lines of Ti, the spherically bent crystal was placed 225 mm from the plasma source and centered at $\lambda = 2.73$ Å (Bragg angle $\theta = 63.3^\circ$). To record the emission, the CCD was placed on the Rowland circle 135.8 mm from the crystal. The spatial resolution of the spectrometer in this configuration was $48 \mu\text{m}$ in the horizontal plane of the target, and the spectral resolution on the CCD was $\lambda/\Delta\lambda \approx 3800$. It should be emphasized that because the crystal had a spherical shape and the detector was placed on the Rowland circle, the spectral resolution was not sensitive to the source size of the plasma.

Figure 1 shows the experimental setup along with FSSR-1D images from four shots from Al-coated Ti foils

TABLE I: Characteristics of four shots including the thickness d of the target Ti foil, the incident laser intensity, the relative $K_{\alpha 2}$ emission intensity, the emission extent Δx of the $K_{\alpha 2}$ line and high-energy satellites, and the transmission of 4510 eV radiation through a cold Ti foil of thickness d . (Because the $K_{\alpha 1}$ line was saturated on the film in shots 1804 and 2211, emission extents and intensities are given only for $K_{\alpha 2}$.)

shot	Ti foil d (μm)	Laser Int. ($\times 10^{18}$ W/cm^2)	$K_{\alpha 2}$ Int.	$K_{\alpha 2}$ Δx (μm)	sat. Δx (μm)	cold Ti transm.
2211	2.0	2.8	0.61	150	100	0.91
1804	12.5	4.0	1.00	250	150	0.54
1801	25	2.0	0.77	200	100	0.29
1806	50	4.0	0.51	100	-	0.09

of various thicknesses. Table I summarizes the characteristics of the target, laser, and measured K_α emission from the four shots shown in Fig. 1. The transmission of 4510 eV radiation through cold Ti foil is also given.

The $K_{\alpha 2}$ emission intensity and the size of the $K_{\alpha 2}$ emission region are correlated in Table I: both increase from the $2 \mu\text{m}$ target to the $12.5 \mu\text{m}$ target, and then decrease with increasing target thickness. This implies that there is an optimal target thickness for maximum K_α intensity and suggests a competition between the number of Ti ions available to fluoresce and the absorption of K_α emission with increasing Ti foil thickness. The measured extents are consistent with high-spatial resolution measurements of Ti K_α yield from buried-layer targets [10]. Also, hot electron temperatures of 100-200 keV were measured using an electron spectrometer aimed at the back surface of the Ti targets; the measured emission extents are consistent with the $\approx 100 \mu\text{m}$ mean free path of few-hundred-keV electrons through Ti at solid density.

Satellites on the high-energy side of the $K_{\alpha 1}$ line are clearly evident in the images in Fig. 1 for all but the $50 \mu\text{m}$ foils; these satellites come from ionized Ti and are discussed in detail below. For now, we point out that the emission region of the high-energy satellites is generally smaller than the emission region of the characteristic $K_{\alpha 2}$ emission. This means that the region of heated Ti is smaller than the region through which the hot electrons responsible for fluorescence travel.

Hydrodynamic simulations [20] of $2 - 25 \mu\text{m}$ Ti foil targets coated with $1 \mu\text{m}$ of Al at the present laser intensities show a shock front moving at $\approx 0.5 \mu\text{m}/\text{ps}$ into the target, heating the material behind it to 100-200 eV. (The fourfold compression of Ti in the simulated shock front is insufficient to pressure-ionize the $3p$ subshell, supporting thermal ionization as the cause of the observed K_α shifts.) Radiation temperatures of 20-50 eV driven by emission from hot Al blowoff plasma run ahead of the shock front by several μm , consistent with the fast radiative heating of laser-irradiated foils described in [11]. However, the spread of both the radiative and shock heating fronts along the target surface is less

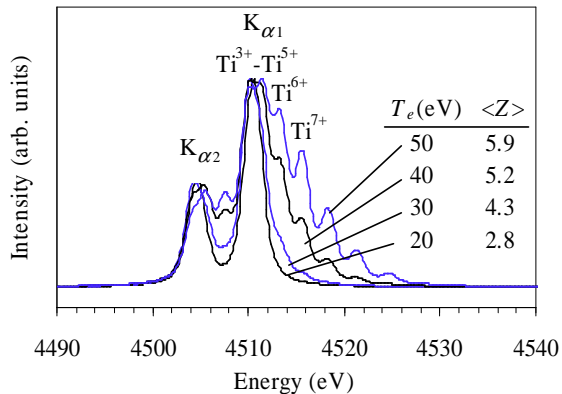


FIG. 2: (Color online) Modeled K_α spectra and self-consistent $\langle Z \rangle$ at various electron temperatures. Increasing ionization gives rise to a blue wing on the characteristic $K_{\alpha 1}$ line and fills in the gap between the cold $K_{\alpha 1}$ and $K_{\alpha 2}$ lines.

than 20 μm . Thus, the heating that causes the measured satellite emission is most likely due to thermalization of 50-100 keV electrons produced in the intense laser field.

To analyze the measured K_α spectra, a self-consistent-field model of ions in dense plasma (MUZE) has been developed. The model generates self-consistent Thomas-Fermi electron densities and potentials in a Wigner-Seitz cell whose radius R_0 is determined by the solid-Ti ion density ($n_i = 5.7 \times 10^{22} \text{cm}^{-3}$). Non-relativistic bound and free wavefunctions are calculated for an average atom in this initial potential and their occupations are determined by varying a chemical potential to ensure the neutrality of the ion cell. A new electron density is determined from these occupations, and a new potential is generated using Poisson's equation. Exchange and correlation effects are added to the potential as prescribed by Rozsnyai in [21]. This procedure is repeated until self-consistent solutions for the wavefunctions and potential are obtained, giving a converged $\langle Z \rangle$. The present model owes much to the development of similar models [21–25].

Next, the average atom is split into individual ions, with potentials and wavefunctions self-consistently optimized for each ion. Approximate relativistic corrections are added to the bound state energies (these account for the splitting between $K_{\alpha 1}$ and $K_{\alpha 2}$) and a single global correction is added to the calculated transition energies so that the cold K_α line matches tabulated values [1]. (In this case, the correction is 26.7 eV, or $\approx 0.5\%$ of the transition energy.) This procedure is similar to that used by House [2] but includes the effects of density on the atomic structure, accounting for continuum lowering by truncating the Rydberg series of $n\ell$ orbitals.

Once the transition energies are calculated, electric dipole oscillator strengths are computed using the average atom wavefunctions and scaled to the transition energies of individual ions. The ion distribution is fixed by enforcing LTE through Saha-Boltzmann equilibrium. Synthetic spectra are constructed using Voigt line shapes

which convolve the nominal instrumental resolution with a Voigt parameter of unity. Line intensities are proportional to the parent ion population, the radiative decay rate, and the statistical weight of the upper level.

To test the model for accuracy, we have compared our results to atomic structure calculations from the relativistic multiconfiguration atomic code FAC [26] for the Ti^{3+} to Ti^{7+} ions. (Neutral Ti to Ti^{2+} are pressure-ionized in MUZE at solid density, so no comparison could be made with the isolated-ion calculations of FAC.) FAC predicts many hundreds of lines from each ion even in the density-restricted configuration space, but the dominant emission features generally retain the dual-peak shape of the characteristic K_α lines and agree with MUZE transition energies to within 1 – 2 eV. Both FAC and MUZE calculate a redshift in moving from Ti^{3+} to Ti^{4+} [2, 6, 7]. We also used the FAC data as input to a collisional-radiative code [27] to confirm that the solid density conditions are sufficient to enforce LTE and that the ionization balance determined by the thermal electron temperature is practically unaffected by hot electron fractions less than a few percent. This last result confirms the conclusions of Ref. [14].

Results of the model for temperatures from 20 to 50 eV are given in Fig. 2. As T_e increases and the Ti atoms ionize, satellite lines emerge on the high-energy side of the $K_{\alpha 1}$ line, giving the appearance of a blue wing, and satellites to the $K_{\alpha 2}$ transition begin to fill in the gap between the cold characteristic lines. The charge states giving rise to selected $K_{\alpha 1}$ satellites are indicated on the figure: lines from Ti^{3+} to Ti^{5+} all lie between 4510 and 4512 eV, while the lines from Ti^{6+} and higher charge states each exhibit a 2 – 3 eV blue shift with each lost $3p$ electron. No appeal to exotic satellites of the kind recently described in Ref. [28] are required in a dense plasma environment because final states of K_α transitions with spectator holes are themselves autoionizing and can simply be taken to belong to a more highly charged ion.

Figure 3 shows a comparison of modeled spectra with measured spectra (lineouts from the central 200 μm portion of the images shown in Fig. 1). The temperatures of the modeled spectra were chosen to give the best fit to the shape of the experimental spectra (normalized to the $K_{\alpha 2}$ line). The K_α temperature diagnostic has a precision of ± 3 -5 eV for $T_e > 25$ eV, as indicated by the dashed lines in the figure showing spectra at $T_e = \pm 5$ eV (changes in the calculated spectra are small for $T_e \leq 25$ eV). The experimental spectra exhibit a clear increase in the intensity of high-energy satellite emission with decreasing target thickness, with up to 8-times-ionized Ti evident in the 2 μm Ti target. The increasing ionization corresponds to increasing thermal temperatures, from less than 25 eV for the thickest foil up to 40 eV for the thinnest. The ion-ion coupling parameters $\Gamma_{ii} = \langle Z \rangle^2 / R_0 k_B T_e$ at these conditions are between 4 and 6 – well within the $\Gamma_{ii} > 1$ limit indicating a strongly coupled plasma.

As noted above, the difference in the spatial extent of the warm-Ti satellites and the characteristic (cold)

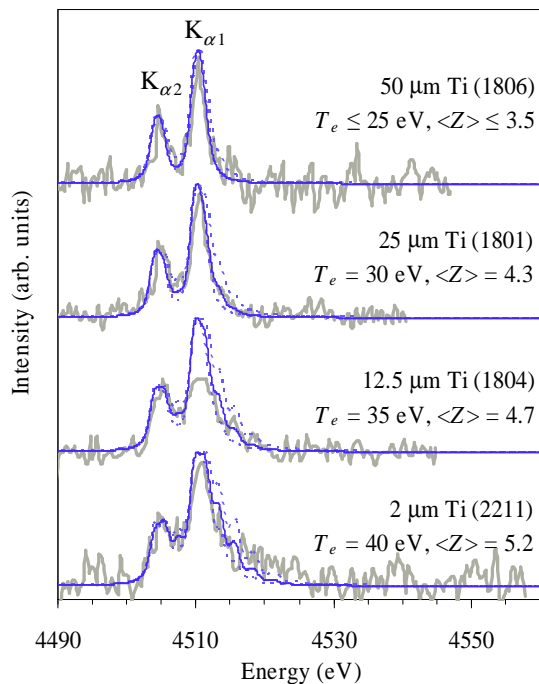


FIG. 3: (Color online) Experimental spectra (gray lines) with relative intensities corresponding to those listed in Table I. The best-fit modeled spectra (solid lines) indicate increasing temperatures with decreasing target thickness. Modeled spectra at temperatures 5 eV above and below the best-fit T_e (dashed lines) indicate the precision of the diagnostic.

K_α emission indicates that the temperature decreases in the radial direction along the surface. Since the lineouts given in Fig. 3 average over that temperature gradient, temperatures higher than the diagnosed T_e may exist. The present measurements also represent a transmission-

modulated average in the direction perpendicular to the surface of the target, along which temperature gradients have previously been observed [13]. If one sets the temperature to be 40 eV in the first $\approx 10 \mu\text{m}$ of the $> 2 \mu\text{m}$ foils and zero in the remainder, the total emission (including absorption) closely resembles the best-fit optically thin spectra given in Fig. 3. Thus the present diagnostics can be taken either to represent an average temperature over the foil thickness or as estimates of the temperature gradient scale length. Buried-layer targets could eliminate the ambiguity.

In summary, we have presented K_α emission measurements taken from the back surface of Al-coated Ti foils of varying thickness irradiated by a high-intensity laser and have introduced a self-consistent-field model for use as a temperature diagnostic of warm, dense matter. Spatial variations in the K_α spectra indicate temperature gradients parallel to the surface of the target material over $\approx 100 \mu\text{m}$ length scales. The high spectral resolution of the measurements has enabled the identification of K_α emission lines from 6 – 8-times ionized Ti, indicating temperatures of at least 40 eV in the first few μm of the tamped Ti target and decreasing average T_e with increasing target thickness.

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